

Semi-spheroidal Quantum Harmonic Oscillator

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(Dated: February 1, 2008)

A new single-particle shell model is derived by solving the Schrödinger equation for a semi-spheroidal potential well. Only the negative parity states of the $Z(z)$ component of the wave function are allowed, so that new magic numbers are obtained for oblate semi-spheroids, semi-sphere and prolate semi-spheroids. The semi-spherical magic numbers are identical with those obtained at the oblate spheroidal superdeformed shape: 2, 6, 14, 26, 44, 68, 100, 140, ... The superdeformed prolate magic numbers of the semi-spheroidal shape are identical with those obtained at the spherical shape of the spheroidal harmonic oscillator: 2, 8, 20, 40, 70, 112, 168 ...

PACS numbers: 03.65.Ge, 21.10.Pc, 31.10.+z,

The spheroidal harmonic oscillator have been used in various branches of Physics. Of particular interest was the famous single-particle Nilsson model [1] very successful in Nuclear Physics and its variants [2, 3, 4] for atomic clusters. Major spherical-shells $N = 2, 8, 20, 40, 58, 92$ have been found [2] in the mass spectra of sodium clusters of N atoms per cluster, and the Clemenger's shell model [3] was able to explain this sequence of spherical magic numbers.

In the present paper we would like to write explicitly the analytical relationships for the energy levels of the spheroidal harmonic oscillator and to derive the corresponding solutions for a semi-spheroidal harmonic oscillator which may be useful to study atomic cluster deposited on planar surfaces.

For spheroidal equipotential surfaces, generated by a potential with cylindrical symmetry the states of the valence electrons were found [3] by using an effective single-particle Hamiltonian with a potential

$$V = \frac{M\omega_0^2 R_0^2}{2} \left[\rho^2 \left(\frac{2+\delta}{2-\delta} \right)^{2/3} + z^2 \left(\frac{2-\delta}{2+\delta} \right)^{4/3} \right] \quad (1)$$

In order to get analytical solutions we shall neglect an additional term proportional to $(\mathbf{l}^2 - \langle \mathbf{l}^2 \rangle_n)$. We plan to include in the future such a term which needs a numerical solution. K. L. Clemenger introduced the deformation δ by expressing the dimensionless two semiaxes (in units of the radius of a sphere with the same volume, $R_0 = r_s N^{1/3}$, where r_s is the Wigner-Seitz radius, 2.117 Å for Na [5, 6]) as

$$a = \left(\frac{2-\delta}{2+\delta} \right)^{1/3} ; \quad c = \left(\frac{2+\delta}{2-\delta} \right)^{2/3} \quad (2)$$

The spheroid surface equation in dimensionless cylindrical coordinates ρ and z is given by

$$\frac{\rho^2}{a^2} + \frac{z^2}{c^2} = 1 \quad (3)$$

where a is the minor (major) semiaxis for prolate (oblate) spheroid and c is the major (minor) semiaxis for prolate (oblate) spheroid. Volume conservation leads to $a^2 c = 1$.

One can separate the variables in the Schrödinger equation, $H\Psi = E\Psi$, written in cylindrical coordinates. As a result the wave function [7, 8] may be written as

$$\Psi(\eta, \xi, \varphi) = \psi_{n_r}^m(\eta) \Phi_m(\varphi) Z_{n_z}(\xi) \quad (4)$$

where each component of the wave function is orthonormalized leading to

$$\Phi_m(\varphi) = e^{im\varphi} / \sqrt{2\pi} \quad (5)$$

$$\begin{aligned} \psi(\eta) &= N_{n_r}^m \eta^{|m|/2} e^{-\eta/2} L_{n_r}^{|m|}(\eta) \\ N_{n_r}^m &= \left(\frac{2n_r!}{\alpha_{\perp}^{2n_r+|m|}} \right)^{1/2} \end{aligned} \quad (6)$$

in which $\eta = R_0^2 \rho^2 / \alpha_{\perp}^2$ and the quantum numbers $m = (n_{\perp} - 2i)$ with $i = 0, 1, \dots$ up to $(n_{\perp} - 1)/2$ for an odd n_{\perp} or to $(n_{\perp} - 2)/2$ for an even n_{\perp} . $L_n^m(x)$ is the associated Laguerre polynomial and the constant $\alpha_{\perp} = \sqrt{\hbar/M\omega_{\perp}}$ has the dimension of a length.

$$\begin{aligned} Z_{n_z}(\xi) &= N_{n_z} e^{-\xi^2} H_{n_z}(\xi) \\ N_{n_z} &= \frac{1}{(\alpha_z \sqrt{\pi} 2^{n_z} n_z!)^{1/2}} \end{aligned} \quad (7)$$

where $\xi = R_0 z / \alpha_z$, $\alpha_z = \sqrt{\hbar/M\omega_z}$, and the main quantum number $n = n_{\perp} + n_z = 0, 1, 2, \dots$

The eigenvalues are

$$E_n = \hbar\omega_{\perp}(n_{\perp} + 1) + \hbar\omega_z(n_z + 1/2) \quad (8)$$

The parity of the Hermite polynomials $H_{n_z}(\xi)$ is given by $(-1)^{n_z}$ meaning that the even order Hermite polynomials are even functions $H_{2n_z}(-\xi) = H_{2n_z}(\xi)$ and the odd order Hermite polynomials are odd functions $H_{2n_z+1}(-\xi) = -H_{2n_z+1}(\xi)$. There is a recurrence relationship $2zH_n = H_{n+1} + 2nH_{n-1}$. One has $H_0 = 1$, $H_1 =$

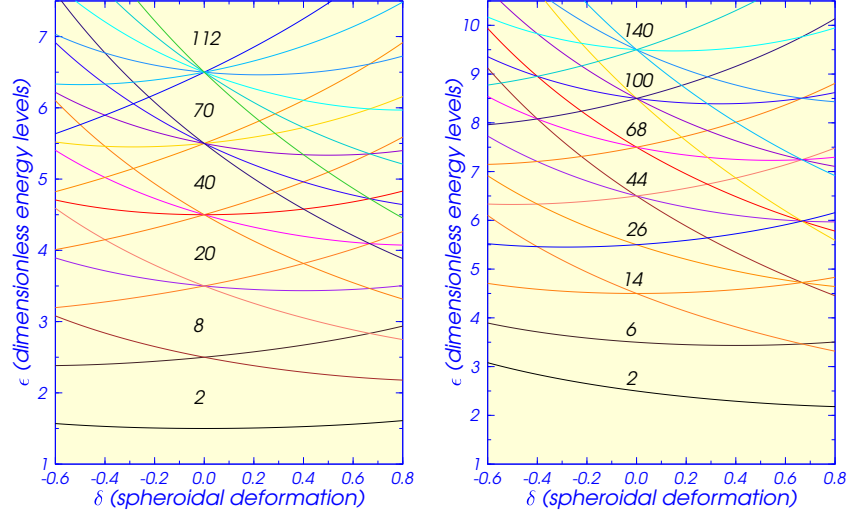


FIG. 1: LEFT: Spheroidal harmonic oscillator energy levels in units of $\hbar\omega_0$ vs. the deformation parameter δ . Only 6 major shells ($N = 0, 1, 2, \dots, 5$) have been considered. Each level is labeled by n, n_\perp quantum numbers and is $(2n_\perp + 2)$ -fold degenerate. The labels are $0, 0; 1, 0, 1, 1; 2, 0, 2, 1, 2, 2; 3, 0, 3, 1, 3, 2, 3, 3; 4, 0, 4, 1, 4, 2, 4, 3, 4, 4$, etc. RIGHT: Semi-spheroidal harmonic oscillator energy levels in units of $\hbar\omega_0$ vs. the deformation coordinate δ . Only 9 major shells ($N = 0, 1, 2, \dots, 8$) have been considered. Each level is labeled by n, n_\perp quantum numbers (with $n_z = n - n_\perp = 1, 3, 5, \dots$ and is $(2n_\perp + 2)$ -fold degenerate. The labels are $1, 0; 2, 1; 3, 2, 3, 0; 4, 3, 4, 1; 5, 4, 5, 2, 5, 0; 6, 5, 6, 3, 6, 1$, etc. The semi-spherical magic numbers are identical with those obtained at the oblate spheroidal superdeformed shape ($\delta = -2/3$): 2, 6, 14, 26, 44, 68, 100, 140, ...

$2z, H_2 = 4z^2 - 2, H_3 = 8z^3 - 12z, H_4 = 16z^4 - 48z^2 + 12, H_5 = 32z^5 - 160z^3 + 120z$, etc.

In units of $\hbar\omega_0$ the eigenvalues, $\epsilon = E/(\hbar\omega_0)$, are given by

$$\epsilon = \frac{2}{(2 - \delta)^{1/3}(2 + \delta)^{2/3}} \left[n + \frac{3}{2} + \delta \left(n_\perp - \frac{n}{2} + \frac{1}{4} \right) \right] \quad (9)$$

For a prolate spheroid, $\delta > 0$, at $n_\perp = 0$ the energy level decreases with deformation except for $n = 0$, but when $n_\perp = n$ it increases. For a given prolate deformation and

a maximum energy ϵ_m , there are n_{min} closed shells and other levels for high-order shells up to n_{max} :

$$n_{min} = \left[(2 - \delta)^{1/3}(2 + \delta)^{2/3}\epsilon_m - \frac{\delta}{2} - 3 \right] \frac{1}{2 + \delta} \quad (10)$$

$$n_{max} = \left[(2 - \delta)^{1/3}(2 + \delta)^{2/3}\epsilon_m - \frac{\delta}{2} - 3 \right] \frac{1}{2 - \delta} \quad (11)$$

and similar formulae for oblate deformations, $\delta < 0$. The low lying energy levels for the six shells (main quantum number $n = 0, 1, 2, 3, 4, 5$) can be seen in figure 1. Each level, labelled by n_\perp, n , may accommodate $2n_\perp + 2$ particles. One has $2 \sum_{n_\perp=0}^n (n_\perp + 1) = (n+1)(n+2)$ nucleons in a completely filled shell characterized by n , and the total number of states of the low-lying $n+1$ shells is $\sum_{n=0}^n (n+1)(n+2) = (n+1)(n+2)(n+3)/3$ leading to the magic numbers 2, 8, 20, 40, 70, 112, 168... for a spherical shape. Besides the important degeneracy at a spherical shape ($\delta = 0$), one also have degeneracies at some superdeformed shapes, e.g. for prolate shapes at the ratio $c/a = (2 + \delta)/(2 - \delta) = 2$ i.e. $\delta = 2/3$. More details may be found in the Table I. The first five shells can reproduce the experimental magic numbers mentioned above; in order to describe the other shells Clemenger introduced the term proportional to $(I^2 - \langle I^2 \rangle_n)$.

Let us consider a particular shape (half of an oblate or prolate spheroid) of a semi-spheroidal cluster deposited on a surface with the z axis perpendicular on the surface and the ρ axis in the surface plane. Then the semi-

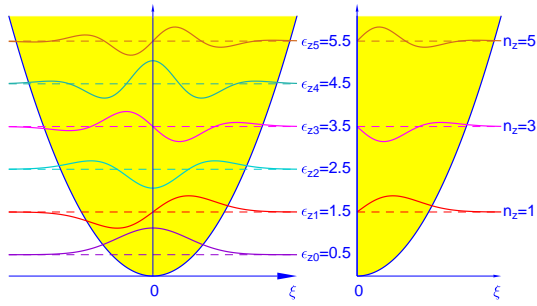


FIG. 2: LEFT: Harmonic oscillator potential $V = V(\xi)$, the wave functions $Z_{n_z} = Z_{n_z}(\xi)$ for $n_z = 0, 1, 2, 3, 4, 5$ and the corresponding contributions to the total energy levels $\epsilon_{n_z} = E_{n_z}/\hbar\omega_z = (n_z + 1/2)$ for spherical shapes, $\delta = 0$. $\xi = zR_0/\sqrt{\hbar/M\omega_z}$. RIGHT: The similar functions for a semi-spherical harmonic oscillator potential. Only negative parity states are retained which are vanishing at $\xi = 0$ where the potential wall is infinitely high.

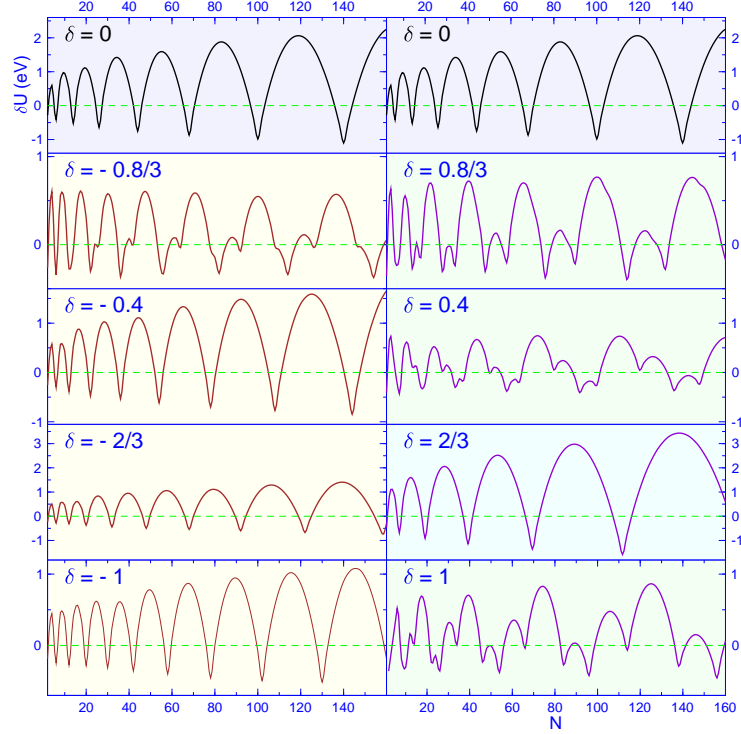


FIG. 3: Variation of shell corrections with N for Na clusters. TOP: $\delta = 0$. The semi-spherical magic numbers are identical with those obtained at the oblate spheroidal superdeformed shape: 2, 6, 14, 26, 44, 68, 100, 140, ... For a prolate superdeformed ($\delta = 2/3$) shape the magic numbers are identical with those obtained at the spherical shape: 2, 8, 20, 40, 70, 112, 168, ... Other magic numbers are given in Table I. Oblate and prolate shapes are considered on the left-hand side and right-hand side, respectively.

spheroidal surface equation is given by

$$\rho^2 = \begin{cases} (a/c)^2(c^2 - z^2) & z \geq 0 \\ 0 & z < 0 \end{cases} \quad (12)$$

The radius of the semi-sphere obtained for the deformation $\delta = 0$ is R_s , given by the volume conservation, $(1/2)(4\pi R_s^3/3) = 4\pi R_0^3/3$, leading to $R_s = 2^{1/3}R_0$. We shall give ρ, z, a, c in units of R_s instead of R_0 . According to the volume conservation, $a^2cR_s^3/2 = R_0^3$ so that $a^2c = 1$. Other kind of shapes obtained from a spheroid by removing less or more than its half (as in the liquid drop calculations [9]) will be considered in the future; in this case it is not possible to obtain analytical solutions.

The new potential well we have to consider in order to solve the quantum mechanical problem is shown in the right-hand side of the figure 2. The potential along the symmetry axis, $V_z(z)$, has a wall of an infinitely large height at $z = 0$, and concerns only positive values of z

$$V_z = \begin{cases} \infty & z = 0 \\ MR_s^2\omega_z^2 z^2/2 & z \geq 0 \end{cases} \quad (13)$$

In this case the wave functions should vanish in the origin, where the potential wall is infinitely high, so that only negative parity Hermite polynomials (n_z odd) should be taken into consideration.

From the energy levels given in figure 1 we have to select only those corresponding to this condition. In this way the former lowest level with $n = 0, n_\perp = 0$ should be excluded. From the two levels with $n = 1$ we can retain the level with $n_\perp = 0$ i.e. $n_z = 1$. This will be the lowest level for the semi-spherical harmonic oscillator and will accommodate $2n_\perp + 2 = 2$ atoms. From the three levels with $n = 2$ only the one with $n_z = n_\perp = 1$ with $2n_\perp + 2 = 4$ degeneracy is retained so that the first two magic numbers at spherical shape ($\delta = 0$) are now 2 followed by 6, etc. Some deformed magic numbers may be found in the Table I and as position of minima in Fig. 3.

Each level, labelled by n_\perp, n , may accommodate $2n_\perp + 2$ particles. When n is an odd number, one should only have even n_\perp in order to select the odd $n_z = n - n_\perp$. The contribution of the shells with odd n to the semi-spherical magic numbers will be

$$\sum_{n_\perp^{even}=0}^{n-1} (2n_\perp + 2) = \frac{(n+1)^2}{2} \quad (14)$$

leading to the sequence 2, 8, 18 for $n = 1, 3, 5$. The contribution of the shells with even n to the semi-spherical

TABLE I: TOP: Deformed magic numbers of the spheroidal harmonic oscillator.
 BOTTOM: Deformed magic numbers of the semi-spheroidal harmonic oscillator.

OBLATE			PROLATE		
δ	a/c	Magic numbers	δ	a/c	Magic numbers
-0.8/3	17/13	2, 8, 18, 20, 34, 38, 58, 64, 92, 100, 136, 148, ...	0.8/3	13/17	2, 8, 20, 22, 42, 46, 76, 82, 124, 134 ...
-0.4	1.5	2, 6, 8, 14, 18, 28, 34, 48, 58, 76, 90, 114, 132, ...	0.4	2/3	2, 8, 10, 22, 26, 46, 54, 66, 84, 96, 114, 138, 156, ...
-2/3	2	2, 6, 14, 26, 44, 68, 100, 140, ...	2/3	0.5	2, 4, 10, 16, 28, 40, 60, 80, 110, 140, ...
-1	3	2, 6, 12, 22, 36, 54, 78, 108, 144, ...	1	1/3	4, 12, 18, 24, 36, 48, 60, 80, 100, 120, 150, ...
-0.8/3	17/13	2, 6, 12, 22, 26, 36, 42, 56, 64, 82, 92, 114, 126, 154, ...	0.8/3	13/17	2, 6, 8, 14, 18, 28, 34, 48, 58, 76, 90, 114, 132, ...
-0.4	1.5	2, 6, 12, 22, 36, 54, 78, 108, 144, ...	0.4	2/3	2, 8, 18, 20, 34, 38, 50, 58, 64, 80, 92, 100, ...
-2/3	2	2, 6, 12, 20, 32, 48, 68, 92, 122, 158, ...	2/3	0.5	2, 8, 20, 40, 70, 112, 168, ...
-1	3	2, 6, 20, 30, 42, 58, 78, 102, 130, ...	1	1/3	2, 8, 10, 14, 22, 26, 46, 54, 66, 84, 96, 114, 138, 156, ...

magic numbers will be

$$\sum_{n_{\perp}^{odd}=1}^{n-1} (2n_{\perp} + 2) = \frac{n(n+2)}{2} \quad (15)$$

which gives the sequence 4, 12, 24 for $n = 2, 4, 6$. This should be interlaced with the preceding one so that the magic numbers will be 2, $2+4=6$, $6+8=14$, $14+12=26$, $26+18=44$, $44+24=68$, as shown at the right-hand side of the Fig. 1.

The equation (9) from the harmonic oscillator, in units of $\hbar\omega_0$ is still valid, but one should only allow the values of n and n_{\perp} for which $n_z = n - n_{\perp} \geq 1$ are odd numbers.

The orthonormalization condition of the Z_{n_z} component of the wave function became

$$\int_0^{+\infty} Z_{n'_z}(z) Z_{n_z}(z) dz = \delta_{n'_z n_z} \quad (16)$$

with $n_z = 1, 3, 5, \dots, n$ for odd n and $n_z = 1, 3, 5, \dots, n-1$ for even n . Consequently the normalization factor is $\sqrt{2}$ times the preceding one

$$\begin{aligned} Z_{n_z}(\xi) &= \sqrt{2} N_{n_z} e^{-\xi^2} H_{n_z}(\xi) \\ N_{n_z} &= \frac{1}{(\alpha_z \sqrt{\pi} 2^{n_z} n_z!)^{1/2}} \end{aligned} \quad (17)$$

For a nucleus with mass number A the shell gap is given by $\hbar\omega_0^0 = 41A^{1/3}$ MeV. For an atomic cluster [10] the single-particle shell gap is given by

$$\hbar\omega_0(N) = \frac{13.72 \text{ eV } \text{\AA}^2}{r_s R_0} \left[1 + \frac{t}{r_s N^{1/3}} \right]^{-2} \quad (18)$$

which is $3.0613N^{-1/3}$ eV in case of Na clusters. Since we consider solely monovalent elements, N in this eq. is the

number of atoms and t denotes the electronic spillout for the neutral cluster according to [10].

The shell correction energy, δU [11], in figure 3 shows minima at the oblate and prolate magic numbers given in the lower part of the table I. The striking result is that the superdeformed prolate magic numbers of the semi-spheroidal shape are identical with those obtained at the spherical shape of the spheroidal harmonic oscillator. We expect that this kind of symmetry will not be present anylonger for the Hamiltonian including the term proportional to $(I^2 - \langle I^2 \rangle_n)$ and/or the more complex equipotential surface we shall study in the future.

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